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The rich and the poor are two locked caskets of which each contains the key to the other.

Karen Blixen (Danish Writer)

1

INTRODUCTORY CONCEPTS

In this Chapter we recapitulate some basic concepts that are used in several chapters that follow. Theorems on electrostatics are included as an introduction to the study of the influence of electric fields on dielectric materials. The solution of Laplace's equation to find the electric field within and without dielectric combinations yield expressions which help to develop the various dielectric theories discussed in subsequent chapters. The band theory of solids is discussed briefly to assist in understanding the electronic structure of dielectrics and a fundamental knowledge of this topic is essential to understand the conduction and breakdown in dielectrics. The energy distribution of charged particles is one of the most basic aspects that are required for a proper understanding of structure of the condensed phase and electrical discharges in gases. Certain theorems are merely mentioned without a rigorous proof and the student should consult a book on electrostatics to supplement the reading.

1.1 A DIPOLE

A pair of equal and opposite charges situated close enough compared with the distance to an observer is called an electric dipole. The quantity

$$\mu = Qd \quad (1.1)$$

where d is the distance between the two charges is called the electric dipole moment. μ is a vector quantity the direction of which is taken from the negative to the positive charge and has the unit of C m. A unit of dipole moment is 1 Debye = 3.33×10^{-30} C m.

1.2 THE POTENTIAL DUE TO A DIPOLE

Let two point charges of equal magnitude and opposite polarity, $+Q$ and $-Q$ be situated d meters apart. It is required to calculate the electric potential at point P , which is situated at a distance of R from the midpoint of the axis of the dipole. Let R_+ and R_- be the distance of the point from the positive and negative charge respectively (fig. 1.1). Let R make an angle θ with the axis of the dipole.

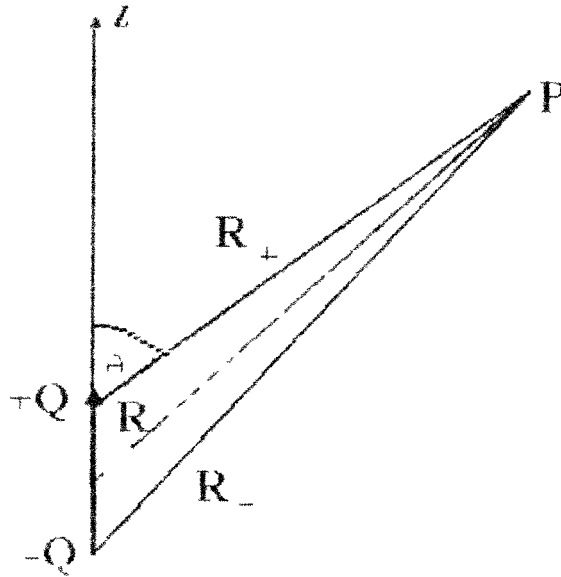


Fig. 1.1 Potential at a far away point P due to a dipole.

The potential at P is equal to

$$\begin{aligned}\phi &= \frac{1}{4\pi\epsilon_0} \left(\frac{Q}{R_+} + \frac{-Q}{R_-} \right) \\ &= \frac{Q}{4\pi\epsilon_0} \left(\frac{1}{R_+} - \frac{1}{R_-} \right)\end{aligned}\tag{1.2}$$

Starting from this equation the potential due to the dipole is

$$\phi \approx \frac{Qd \cos \theta}{4\pi\epsilon_0 R^2}\tag{1.3}$$

Three other forms of equation (1.3) are often useful. They are

$$\phi = \frac{\boldsymbol{\mu} \cdot \mathbf{a}_R}{4\pi\epsilon_0 R^2} \quad (1.4)$$

$$\phi = \frac{\boldsymbol{\mu} \cdot \mathbf{R}}{4\pi\epsilon_0 R^3} \quad (1.5)$$

$$\phi = \frac{\mu z}{4\pi\epsilon_0 R^3} \quad (1.6)$$

The potential due to a dipole decreases more rapidly than that due to a single charge as the distance is increased. Hence equation (1.3) should not be used when $R \approx d$. To determine its accuracy relative to eq. (1.2) consider a point along the axis of the dipole at a distance of $R=d$ from the positive charge. Since $\theta = 0$ in this case, $\phi = Qd/4\pi\epsilon_0 (1.5d)^2 = Q/9\pi\epsilon_0 d$ according to (1.3). If we use equation (1.2) instead, the potential is $Q/8\pi\epsilon_0 d$, an error of about 12%.

The electric field due to a dipole in spherical coordinates with two variables (r, θ) is given as:

$$\begin{aligned} \mathbf{E} &= \frac{-\partial\phi}{\partial r} \mathbf{a}_r - \frac{1}{r} \frac{\partial\phi}{\partial\theta} \mathbf{a}_\theta \\ &= \mathbf{E}_r \mathbf{a}_r + \mathbf{E}_\theta \mathbf{a}_\theta \end{aligned} \quad (1.7)$$

Partial differentiation of equation (1.3) leads to

$$\mathbf{E}_r = \frac{Qd \cos\theta}{2\pi\epsilon_0 R^3} \quad (1.8)$$

$$\mathbf{E}_\theta = \frac{Qd \sin\theta}{4\pi\epsilon_0 R^3} \quad (1.9)$$

Equation (1.7) may be written more concisely as:

$$\mathbf{E} = -\nabla\phi \quad (1.10)$$

Substituting for ϕ from equation (1.5) and changing the variable to r from R we get

$$\mathbf{E} = -\frac{\nabla\boldsymbol{\mu} \cdot \mathbf{r}}{4\pi\epsilon_0 r^3} \quad (1.11)$$

$$= -\frac{\boldsymbol{\mu} \cdot \mathbf{r}}{4\pi\epsilon_0 r^3} \nabla \frac{1}{r^3} - \frac{1}{4\pi\epsilon_0 r^3} \nabla \boldsymbol{\mu} \cdot \mathbf{r} \quad (1.12)$$

We may now make the substitution

$$\nabla \frac{1}{r^3} = -\frac{3}{r^4} \mathbf{a}_r = -\frac{3\mathbf{r}}{r^5}$$

$$\nabla \boldsymbol{\mu} \cdot \mathbf{r} = \boldsymbol{\mu} \mathbf{a}_\theta$$

Equation (1.12) now becomes

$$\mathbf{E} = \left[\frac{3\boldsymbol{\mu} \cdot \mathbf{r}}{r^5} \mathbf{r} - \frac{\boldsymbol{\mu}}{r^3} \right] \frac{1}{4\pi\epsilon_0} \quad (1.13)$$

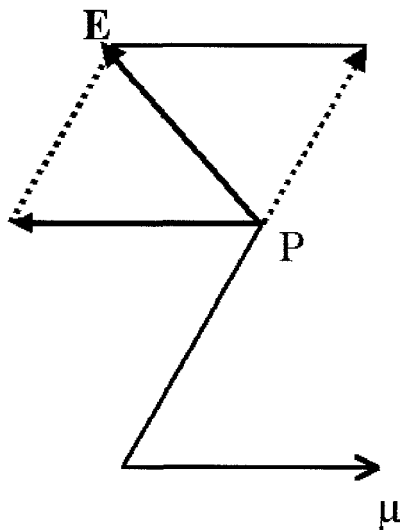


Fig. 1.2 The two components of the electric field due to a dipole with moment $\boldsymbol{\mu}$.

The electric field at P has two components. The first term in equation (1.13) is along the radius vector (figure 1.2) and the second term is along the dipole moment. Note that the second term is anti-parallel to the direction of μ .

In tensor notation equation (1.13) is expressed as

$$\mathbf{E} = \mathbf{T}\mu \quad (1.14)$$

where $\mathbf{T}$ is the tensor $3\mathbf{r}\mathbf{r}\mathbf{r}^{-5} - r^{-3}$.

1.3 DIPOLE MOMENT OF A SPHERICAL CHARGE

Consider a spherical volume in which a negative charge is uniformly distributed and at the center of which a point positive charge is situated. The net charge of the system is zero. It is clear that, to counteract the Coulomb force of attraction the negative charge must be in continuous motion. When the charge sphere is located in a homogeneous electric field $\mathbf{E}$, the positive charge will be attracted to the negative plate and vice versa. This introduces a dislocation of the charge centers, inducing a dipole moment in the sphere.

The force due to the external field on the positive charge is

$$\mathbf{F} = Ze\mathbf{E} \quad (1.15)$$

in which Ze is the charge at the nucleus. The Coulomb force of attraction between the positive and negative charge centers is

$$F' = \frac{ze \cdot e_1}{4\pi\epsilon_0 x^2} \quad (1.16)$$

in which e_1 is the charge in a sphere of radius x and x is the displacement of charge centers. Assuming a uniform distribution of electronic charge density within a sphere of atomic radius R the charge e_1 may be expressed as

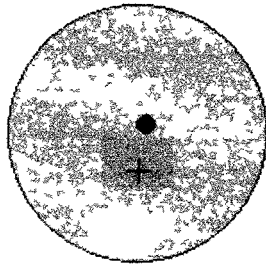
$$e_1 = \frac{ze \cdot x^3}{R^3} \quad (1.17)$$

Substituting equation (1.17) in (1.16) we get

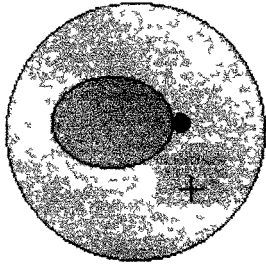
$$F' = \frac{(ze)^2 x}{4\pi\epsilon_0 R^3} \quad (1.18)$$

If the applied field is not high enough to overcome the Coulomb force of attraction, as will be the case under normal experimental conditions, an equilibrium will be established when $F = F'$ viz.,

$$ze \cdot E = \frac{(ze)^2 x}{4\pi\epsilon_0 R^3} \quad (1.19)$$



The center of the negative charge coincides with the nucleus



In the presence of an Electric field the center of the electronic charge is shifted towards the positive electrode inducing a dipole moment in the atom.

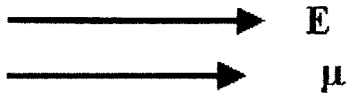


Fig. 1.3 Induced dipole moment in an atom. The electric field shifts the negative charge center to the left and the displacement, x , determines the magnitude.

The displacement is expressed as

$$x = \frac{4\pi\epsilon_0 R^3}{ze} E \quad (1.20)$$

The dipole moment induced in the sphere is therefore

$$\mu_{ind} = zex = 4\pi\epsilon_0 R^3 E \quad (1.21)$$

According to equation (1.21) the dipole moment of the spherical charge system is proportional to the radius of the sphere, at constant electric field intensity. If we define a quantity, polarizability, α , as the induced dipole moment per unit electric field intensity, then α is a scalar quantity having the units of Farad meter. It is given by the expression

$$\alpha = \frac{\mu_{ind}}{E} = 4\pi\epsilon_0 R^3 \quad (1.22)$$

1.4 LAPLACE'S EQUATION

In spherical co-ordinates (r,θ,φ) Laplace's equation is expressed as

$$\nabla^2 V = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial V}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial V}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 V}{\partial \phi^2} = 0 \quad (1.23)$$

If there is symmetry about φ co-ordinate, then equation (1.23) becomes

$$\frac{\partial}{\partial r} \left(r^2 \frac{\partial V}{\partial r} \right) + \frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial V}{\partial \theta} \right) = 0 \quad (1.24)$$

The general solution of equation (1.24) is

$$V = \left(Ar + \frac{B}{r^2} \right) \cos \theta \quad (1.25)$$

in which A and B are constants which are determined by the boundary conditions. It is easy to verify the solution by substituting equation (1.25) in (1.24).

The method of finding the solution of Laplace's equation in some typical examples is shown in the following sections.

1.4.1 A DIELECTRIC SPHERE IMMERSED IN A DIFFERENT MEDIUM

A typical problem in the application of Laplace's equation towards dielectric studies is to find the electric field inside an uncharged dielectric sphere of radius R and a dielectric constant ϵ_2 . The sphere is situated in a dielectric medium extending to infinity and having a dielectric constant of ϵ_1 and an external electric field is applied along Z direction, as shown in figure 1.4. Without the dielectric the potential at a point is, $\phi = -E Z$.

There are two distinct regions: (1) Region 1 which is the space outside the dielectric sphere; (2) Region 2 which is the space within. Let the subscripts 1 and 2 denote the two regions, respectively. Since the electric field is along Z direction the potential in each region is given by equation (1.24) and the general solution has the form of equation (1.25).

Thus the potential within the sphere is denoted by ϕ_2 . The solutions are:

Region 1:

$$\phi_1 = \left(A_1 r + \frac{B_1}{r^2} \right) \cos \theta \quad (1.26)$$

Region 2:

$$\phi_2 = \left(A_2 r + \frac{B_2}{r^2} \right) \cos \theta \quad (1.27)$$

To determine the four constants A_1 B_2 the following boundary conditions are applied.

- (1) Choosing the center of the sphere as the origin, ϕ_2 is finite at $r = 0$. Hence $B_2 = 0$ and

$$\phi_2 = A_2 r \cos \theta \quad (1.28)$$

- (2) In region 1, at $r \rightarrow \infty$, ϕ_1 is due to the applied field is only since the influence of the sphere is negligible. i.e.,

$$d\phi_1 = -E dz \quad (1.29)$$

which leads to

$$\phi_1 = -E z \quad (1.30)$$

Since $r \cos \theta = z$ equation (1.30) becomes

$$\phi_1 = -E r \cos \theta \quad (1.31)$$

Substituting this in equation (1.26) yields $A_1 = -E$, and

$$\phi_1 = \left(-E r + \frac{B_1}{r^2} \right) \cos \theta \quad (1.32)$$

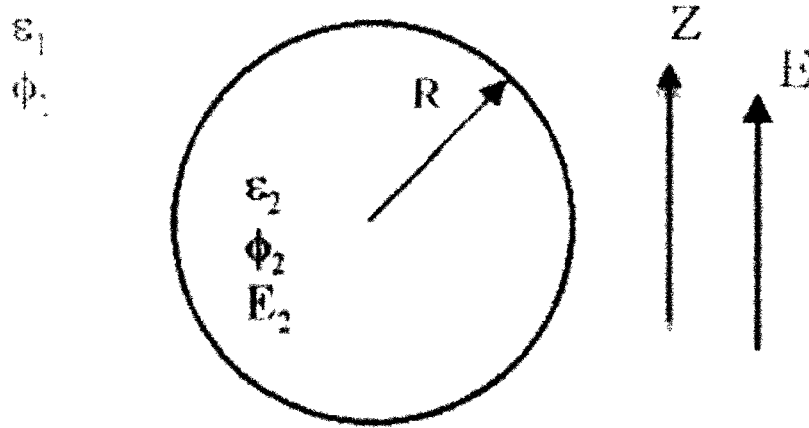


Fig. 1.4 Dielectric sphere embedded in a different material and an external field is applied.

- (3) The normal component of the flux density is continuous across the dielectric boundary, *i.e.*, at $r = R$,

$$\epsilon_o \epsilon_2 E_2 = \epsilon_o \epsilon_1 E_1 \quad (1.33)$$

resulting in

$$\left(\epsilon_2 \frac{\partial \phi_2}{\partial r} \right)_{r=R} = \left(\epsilon_1 \frac{\partial \phi_1}{\partial r} \right)_{r=R} \quad (1.34)$$

Differentiating equations (1.28) and (1.32) and substituting in (1.34) yields

$$\varepsilon_2 A_2 = -\varepsilon_1 \left(E + \frac{2B_1}{R^3} \right) \quad (1.35)$$

leading to

$$B_1 = \frac{-R^3(\varepsilon_2 A_2 + \varepsilon_1 E)}{2\varepsilon_1} \quad (1.36)$$

(4) The tangential component of the electric field must be the same on each side of the boundary, *i.e.*, at $r = R$ we have $\phi_1 = \phi_2$. Substituting this condition in equation (1.26) and (1.28) and simplifying results in

$$A_2 R = \frac{B_1}{R^2} - ER \quad (1.37)$$

Further simplification yields

$$B_1 = R^3(A_2 + E) \quad (1.38)$$

Equating (1.36) and (1.38), A_2 is obtained as

$$A_2 = -\frac{3\varepsilon_1}{2\varepsilon_1 + \varepsilon_2} E \quad (1.39)$$

Hence

$$B_1 = R^3 \left(\frac{\varepsilon_2 - \varepsilon_1}{2\varepsilon_1 + \varepsilon_2} \right) E \quad (1.40)$$

Substituting equation (1.39) in (1.28) the potential within the dielectric sphere is

$$\phi_2 = -\frac{3\varepsilon_1}{2\varepsilon_1 + \varepsilon_2} Ez \quad (1.41)$$

From equation (1.41) we deduce that the potential inside the sphere varies only with z , *i.e.*, the electric field within the sphere is uniform and directed along E . Further,

$$E_2 = -\frac{\partial \phi_2}{\partial z} = \frac{3\varepsilon_1}{2\varepsilon_1 + \varepsilon_2} \mathbf{E} \quad (1.42)$$

(a) If the inside of the sphere is a cavity, *i.e.*, $\varepsilon_2=1$ then

$$\mathbf{E}_2 = \frac{3\varepsilon_1}{2\varepsilon_1 + 1} \mathbf{E} \quad (1.43)$$

resulting in an enhancement of the field.

(b) If the sphere is situated in a vacuum, *ie.*, $\varepsilon_1=1$ then

$$\mathbf{E}_2 = \frac{3}{2 + \varepsilon_2} \mathbf{E} \quad (1.44)$$

resulting in a reduction of the field inside.

Substituting for A_1 and B_1 in equation (1.26) the potential in region (1) is expressed as

$$\phi_1 = \left[\frac{(\varepsilon_2 - \varepsilon_1) R^3}{(2\varepsilon_1 + \varepsilon_2) r^3} - 1 \right] EZ \quad (1.45)$$

The changes in the potentials ϕ_1 and ϕ_2 are obviously due to the apparent surface charges on the dielectric. If we represent these changes as $\Delta\phi_1$ and $\Delta\phi_2$ in region 1 and 2 respectively by defining

$$\Delta\phi_1 = \phi + \phi_1 \quad (1.46)$$

$$\Delta\phi_2 = \phi + \phi_2 \quad (1.47)$$

where ϕ is the potential applied in the absence of the dielectric sphere, then

$$\Delta\phi_1 = \frac{\varepsilon_2 - \varepsilon_1}{2\varepsilon_1 + \varepsilon_2} \frac{R^3}{r^3} EZ \quad (1.48)$$

$$\Delta\phi_2 = \frac{\epsilon_2 - \epsilon_1}{2\epsilon_1 + \epsilon_2} EZ \quad (1.49)$$

Fig. 1.5 shows the variation of $\mathbf{E}_2$ for different values of ϵ_2 with respect to ϵ_1 .

The increase in potential within the sphere, equation (1.49), gives rise to an electric field

$$\frac{\Delta\phi_2}{\Delta z} = \Delta\mathbf{E} = -\frac{\epsilon_2 - \epsilon_1}{2\epsilon_1 + \epsilon_2} \mathbf{E} \quad (1.50)$$

The total electric field within the sphere is

$$\mathbf{E}_2 = \Delta\mathbf{E} + \mathbf{E} \quad (1.51)$$

$$= \frac{3\epsilon_1}{2\epsilon_1 + \epsilon_2} \mathbf{E} \quad (1.52)$$

Equation (1.52) agrees with equation (1.42) verifying the correctness of the solution.

1.4.2 A RIGID DIPOLE IN A CAVITY WITHIN A DIELECTRIC

We now consider a hollow cavity in a dielectric material, with a rigid dipole at the center and we wish to calculate the electric field within the cavity. The cavity is assumed to be spherical with a radius R . A dipole is defined as rigid if its dipole moment is not changed due to the electric field in which it is situated. The material has a dielectric constant ϵ (Fig. 1.6).

The boundary conditions are:

- (1) $(\phi_1)_{r \rightarrow \infty} = 0$ because the influence of the dipole decreases with increasing distance from it according to equation (1.3). Substituting this boundary condition in equation (1.26) gives $A_1=0$ and therefore

$$\phi_1 = \frac{B_1 \cos\theta}{r^2} \quad (1.53)$$

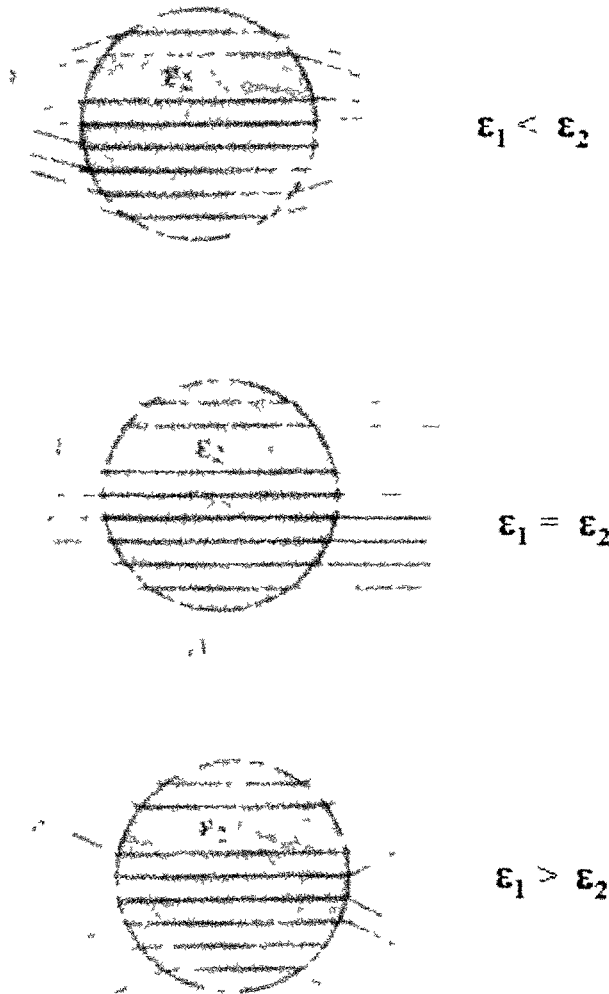


Fig. 1.5 Electric field lines in two dielectric media. The influence of relative dielectric constants of the two media are shown. (a) $\epsilon_1 < \epsilon_2$ (b) $\epsilon_1 = \epsilon_2$ (c) $\epsilon_1 > \epsilon_2$

(2) At any point on the boundary of the sphere the potential is the same whether we approach the point from infinity or the center of the sphere. This condition gives

$$(\phi_1)_{r=R} = (\phi_2)_{r=R} \quad (1.54)$$

leading to

$$B_1 = A_2 R^3 + B_2 \quad (1.55)$$

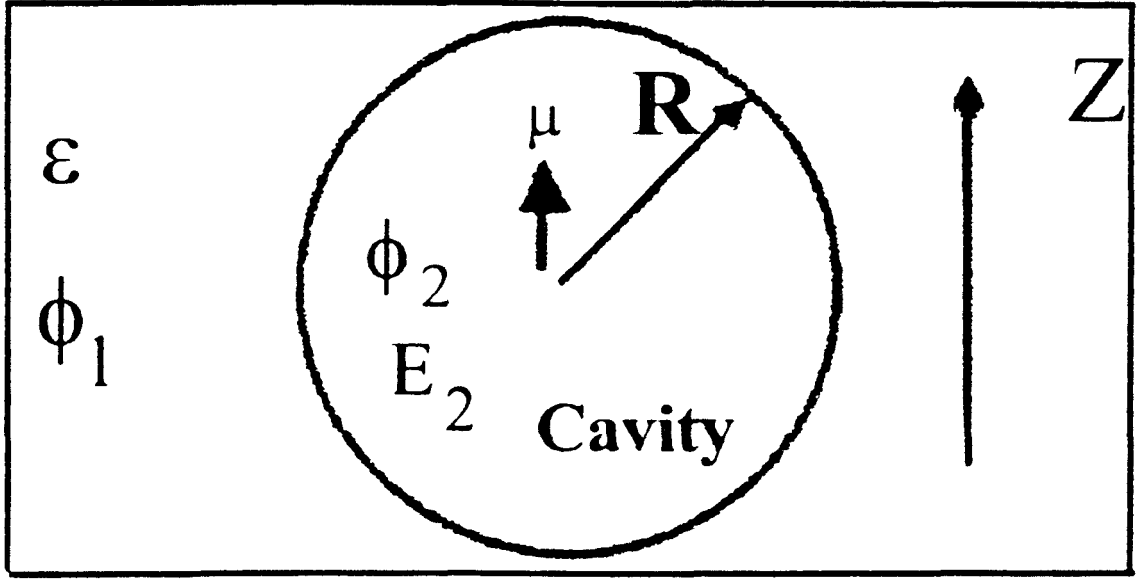


Fig. 1.6 A rigid dipole at the center of a cavity in a dielectric material. There is no applied electric field.

- (3) The normal component of the flux density across the boundary is continuous, expressed as

$$\left(\frac{\partial \phi_2}{\partial r} \right)_{r=R} = \epsilon \left(\frac{\partial \phi_1}{\partial r} \right)_{r=R} \quad (1.56)$$

Applying this condition to the pair of equations (1.26) and (1.27) leads to

$$A_2 = \frac{2}{R^3} (B_2 - B_1 \epsilon) \quad (1.57)$$

- (4) If the boundary of the sphere is moved far away *i.e.*, $R \rightarrow \infty$ the potential at any point is given by equation (1.3),

$$(\phi_2)_{R \rightarrow \infty} = \frac{\mu \cos \theta}{4\pi \epsilon_0 r^2} \quad (1.58)$$

and

$$A_2 = 0 \quad (1.59)$$

Substituting equations (1.58) and (1.59) in equation (1.27) results in

$$B_2 = \frac{\mu}{4\pi\epsilon_o} \quad (1.60)$$

Equation (1.57) now becomes

$$A_2 = \frac{2\mu}{4\pi\epsilon_o R^3} \frac{(1-\epsilon)}{(1+2\epsilon)} \quad (1.61)$$

Substituting equation (1.61) in (1.55) gives

$$B_1 = \frac{\mu}{4\pi\epsilon_o} \left(\frac{3}{1+2\epsilon} \right) \quad (1.62)$$

For convenience the other two constants are collected here:

$$B_2 = \frac{\mu}{4\pi\epsilon_o} \quad (1.60)$$

$$A_1 = 0$$

The potential in the two regions are:

$$\phi_1 = \frac{\mu \cos \theta}{4\pi\epsilon_o r^2} \left(\frac{3}{2\epsilon+1} \right) \quad (1.63)$$

$$\phi_2 = \frac{\mu \cos \theta}{4\pi\epsilon_o} \left[\frac{1}{r^2} + \frac{2r(1-\epsilon)}{R^3(2\epsilon+1)} \right] \quad (1.64)$$

Let ϕ_r be the potential at r due to the dipole in vacuum. The change in potential in the presence of the dielectric sphere is due to the presence of apparent charges on the walls of the sphere. These changes are:

$$\Delta\phi_1 = \phi_1 - \phi_r$$

$$= \frac{2(1-\varepsilon)}{2\varepsilon+1} \frac{\mu \cos\theta}{4\pi\varepsilon_0 r^2} \quad (1.65)$$

$$\Delta\phi_2 = \frac{2(1-\varepsilon)}{4\pi\varepsilon_0 R^3 (2\varepsilon+1)} \mu r \cos\theta \quad (1.66)$$

Since ε is greater than unity equations (1.63) and (1.64) show that there is a decrease in potential in both regions. The apparent surface charge has a dipole moment μ_a given by

$$\mu_a = \frac{2(1-\varepsilon)}{2\varepsilon+1} \mu \quad (1.67)$$

Equation (1.66) shows that the electric field in the cavity has increased by **R**, called the reaction field according to

$$\mathbf{R} = \frac{2(\varepsilon-1)}{4\pi\varepsilon_0 R^3 (2\varepsilon+1)} \mu \quad (1.68)$$

It is interesting to calculate the approximate magnitude of this field at molecular level. Substituting $\mu = 1$ Debye $= 3.3 \times 10^{-30}$ C m, $R = 1 \times 10^{-10}$ m, and $\varepsilon = 3$, the reaction field is of the order of 10^{10} V/m which is very high indeed. The field reduces rapidly with distance, at $R = 1 \times 10^{-9}$ m, it is 10^7 V/m, a reduction by a factor of 1000. This is due to the fact that the reaction field changes according to the third power of R .

The converse problem of a dipole situated in a dielectric sphere which is immersed in vacuum may be solved similarly and the reaction field will then become

$$\mathbf{R} = \frac{2(1-\varepsilon)\mu}{4\pi\varepsilon_0 \varepsilon R^3 (2+\varepsilon)} \quad (1.69)$$

If the dipole is situated in a medium that has a dielectric constant of ε_2 and the dielectric constant of region 1 is denoted by ε_1 the reaction field within the sphere is given by

$$\mathbf{R} = \frac{2(\varepsilon_1 - \varepsilon_2)}{4\pi\varepsilon_0\varepsilon_2r^3(2\varepsilon_1 + \varepsilon_2)}\mu \quad (1.70)$$

It is easy to see that the relative values of ε_1 and ε_2 determine the magnitude of the reaction field. The reaction field is parallel to the dipole moment.

The general result for a dipole within a sphere of dielectric constant ε_2 surrounded by a second dielectric medium ε_1 is

$$\phi_1 = \frac{\mu \cos \theta}{4\pi\varepsilon_0\varepsilon_2r^2} \left(\frac{3\varepsilon_2}{\varepsilon_2 + 2\varepsilon_1} \right)$$

$$\phi_2 = \frac{\mu \cos \theta}{4\pi\varepsilon_0\varepsilon_2} \left[\frac{1}{r^2} + \frac{2r(\varepsilon_2 - \varepsilon_1)}{R^3(\varepsilon_2 + 2\varepsilon_1)} \right]$$

If $\varepsilon_2 = 1$ then these equations reduce to equations (1.63) and (1.64). If $R \rightarrow \infty$ then ϕ_2 reduces to a form given by (1.3).

1.4.3 FIELD IN A DIELECTRIC DUE TO A CONDUCTING INCLUSION

When a conducting sphere is embedded in a dielectric and an electric field $\mathbf{E}$ is applied the field outside the sphere is modified. The boundary conditions are:

(1) At $r \rightarrow \infty$ the electric field is due to the external source and $\phi_1 \rightarrow -Ercos\theta$.

Substituting this condition in equation (1.26) gives $A_1 = -E$ and therefore

$$\phi_1 = \left(-Er + \frac{B_1}{r^2} \right) \cos \theta \quad (1.71)$$

(2) Since the sphere is conducting there is no field within. Let us assume that the surface potential is zero. *i.e.*,

$$(\phi_1)_{r=R} = (\phi_2)_{r=R} = 0 \quad (1.72)$$

This condition when applied to equation (1.26) gives

$$\left(-ER + \frac{B_1}{R^2}\right)\cos\theta = 0 \quad (1.73)$$

Equation (1.73) is applicable for all values of θ and therefore

$$B_1 = ER^3 \quad (1.74)$$

The potential in region 1 is obtained as

$$\phi_1 = \left(-Er + \frac{ER^3}{r^2}\right)\cos\theta \quad (1.75)$$

We note that the presence of the inclusion increases the potential by an amount given by the second term of the eq. (1.75). Comparing it with equation (1.3) it is deduced that the increase in potential is equivalent to $4\pi\epsilon_0$ times the potential due to a dipole of moment of value ER^3 .

1.5 THE TUNNELING PHENOMENON

Let an electron of total energy ϵ eV be moving along x direction and the forces acting on it are such that the potential energy in the region $x < 0$ is zero (fig. 1.7). So its energy is entirely kinetic. It encounters a **potential barrier** of height ϵ_{pot} which is greater than its energy. According to classical theory the electron cannot overcome the potential barrier and it will be reflected back, remaining on the left side of the barrier. However according to quantum mechanics there is a finite probability for the electron to appear on the right side of the barrier.

To understand the situation better let us divide the region into three parts:

- (1) Region I from which the electron approaches the barrier.
- (2) Region II of thickness d which is the barrier itself.
- (3) Region III to the right of the barrier.

The Schrödinger's equation may be solved for each region separately and the constants in each region is adjusted such that there are no discontinuities as we move from one region to the other.

A traveling wave encountering an obstruction will be partly reflected and partly transmitted. The reflected wave in region I will be in a direction opposite to that of the incident wave and a lower amplitude though the same frequency. The superposition of the two waves will result in a standing wave pattern. The solution in this region is of the type[†]

$$\psi_1(x) = A_1 \exp\left(\frac{jpx}{\hbar}\right) + A_2 \exp\left(-\frac{jpx}{\hbar}\right) \quad (1.76)$$

where we have made the substitutions:

$$\hbar = \frac{h}{2\pi}; \quad \varepsilon = \frac{1}{2}mv^2; \quad p = mv = \sqrt{2m\varepsilon} \quad (1.77)$$

The first term in equation (1.76) is the incident wave, in the x direction; the second term is the reflected wave, in the $-x$ direction.

Within the barrier the wave function decays exponentially from $x = 0$ to $x = d$ according to:

$$\psi_{II} = A_2 \exp\left(-\frac{p_1 x}{\hbar}\right) + B_2 \exp\left(-\frac{p_1 x}{\hbar}\right); \quad 0 \leq x \leq d \quad (1.78)$$

$$p_1 = \sqrt{2m(\varepsilon_{pot} - \varepsilon)} \quad (1.79)$$

Since $\varepsilon_{pot} > \varepsilon$ the probability density is real within the region $0 \leq x \leq d$ and the density decreases exponentially with the barrier thickness. The central point is that in the case of a sufficiently thin barrier (< 1 nm) we have a finite, though small, probability of finding the electron on the right side of the barrier. This phenomenon is called the **tunneling effect**.

The relative probability that tunneling will occur is expressed as the **transmission co-efficient** and this is strongly dependent on the energy difference ($\varepsilon_{pot} - \varepsilon$) and d . After tedious mathematical manipulations we get the **transmission co-efficient** as

$$T = \exp(-2p_1d) \quad (1.80)$$

in which p_1 has already been defined in connection with eq. (1.79). A co-efficient of $T=0.01$ means that 1% of the electrons impinging on the barrier will tunnel through. The remaining 99% will be reflected.

The tunnel effect has practical applications in the tunnel diode, Josephson junction and scanning tunneling microscope.

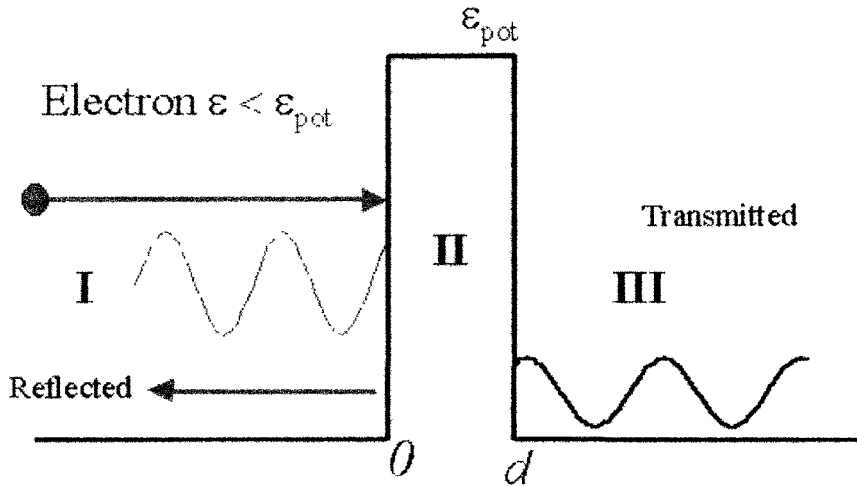


Fig. 1.7 An electron moving from the left has zero potential energy. It encounters a barrier of ϵ_{pot} Volts and the electron wave is partly reflected and partly transmitted. The transmitted wave penetrates the barrier and appears on the right of the barrier². (with permission of McGraw Hill Ltd., Boston).

1.6 BAND THEORY OF SOLIDS

A brief description of the band theory of solids is provided here. For greater details standard text books may be consulted.

1.6.1 ENERGY BANDS IN SOLIDS

If there are N atoms in a solid sufficiently close we cannot ignore the interaction between them, that is, the wave functions associated with the valence electrons can not be treated as remaining distinct. This means that the N wave functions combine in $2N$ different ways. The wave functions are of the form

$$\begin{aligned}
\psi_1 &= \psi_1^i + \psi_2^i + \psi_3^i + \dots + \psi_N^i \\
\psi_2 &= \psi_1^i + \psi_2^i + \psi_3^i + \dots - \psi_N^i \\
&\dots \\
\psi_{2N-1} &= \psi_1^i - \psi_2^i + \psi_3^i + \dots + \psi_N^i \\
\psi_{2N} &= -\psi_1^i + \psi_2^i + \psi_3^i + \dots + \psi_N^i
\end{aligned}
\tag{1.81}$$

Each orbital is associated with a particular energy and we have $2N$ energy levels into which the isolated level of the electron splits. Recalling that $N \approx 10^{28}$ atoms per m^3 the energy levels are so close that they are viewed as an energy band. The energy bands of a solid are separated from each other in the same way that energy levels are separated from each other in the isolated atom.

1.6.2 THE FERMI LEVEL

In a metal the various energy bands overlap resulting in a single band which is partially full. At a temperature of zero Kelvin the highest energy level occupied by electrons is known as the Fermi level and denoted by ϵ_F . The reference energy level for *Fermi energy* is the bottom of the energy band so that the *Fermi energy* has a positive value. The probability of finding an electron with energy ϵ is given by the Fermi-Dirac statistics according to which we have

$$P(\epsilon) = \frac{1}{1 + \exp\left[\frac{\epsilon - \epsilon_F}{kT}\right]}
\tag{1.81}$$

At $\epsilon = \epsilon_F$ the probability of finding the electron is $\frac{1}{2}$ for all values of kT so that we may also define the Fermi Energy at temperature T as that energy at which the probability of finding the electron is $\frac{1}{2}$. The occupied energy levels and the probability are shown for four temperatures in figure (1.8). As the temperature increases the probability extends to higher energies. It is interesting to compare the probability given by the Boltzmann classical theory:

$$P(\epsilon) = A \exp\left(\frac{-\epsilon}{kT}\right)
\tag{1.82}$$

The fundamental idea that governs these two equations is that, in classical physics we do not have to worry about the number of electrons having the same energy. However in

quantum mechanics there cannot be two electrons having the same energy due to Pauli's exclusion principle. For $(\varepsilon - \varepsilon_F) \gg kT$ equation (1.81) may be approximated to

$$P(\varepsilon) = \exp\left(-\frac{\varepsilon - \varepsilon_F}{kT}\right) \quad (1.83)$$

which has a similar form to the classical equation (1.82).

The elementary band theory of solids, when applied to semi-conductors and insulators, results in a picture in which the conduction band and the valence bands are separated by a forbidden energy gap which is larger in insulators than in semi-conductors. In a perfect dielectric the forbidden gap cannot harbor any electrons; however presence of impurity centers and structural disorder introduces localized states between the conduction band and the valence band. Both holes and electron traps are possible³.

Fig. 1.9 summarizes the band theory of solids which explains the differences between conductors, semi-conductors and insulators. A brief description is provided below.

A: In metals the filled valence band and the conduction band are separated by a forbidden band which is much smaller than kT where k is the Boltzmann constant and T the absolute temperature.

B: In semi-conductors the forbidden band is approximately the same as kT .

C: In dielectrics the forbidden band is several electron volts larger than kT . Thermal excitation alone is not enough for valence electrons to jump over the forbidden gap.

D: In p-type semi-conductor acceptors extend the valence band to lower the forbidden energy gap.

E: In n-type semi-conductor donors lower the unfilled conduction band again lowering the forbidden energy gap.

F: In p-n type semi-conductor both acceptors and donors lower the energy gap.

An important point to note with regard to the band theory is that the theory assumes a periodic crystal lattice structure. In amorphous materials this assumption is not justified and the modifications that should be incorporated have a bearing on the theoretical magnitude of current. The fundamental concept of the individual energy levels transforming into bands is still valid because the interaction between neighboring atoms is still present in the amorphous material just as in a crystalline lattice. Owing to irregularities in the lattice the edges of the energy bands lose their sharp character and become rather foggy with a certain number of allowed states appearing in the tail of each

band. If the tail of the valence band overlaps the tail of the conduction band then the material behaves as a semi-conductor⁺ (fig. 1.10).

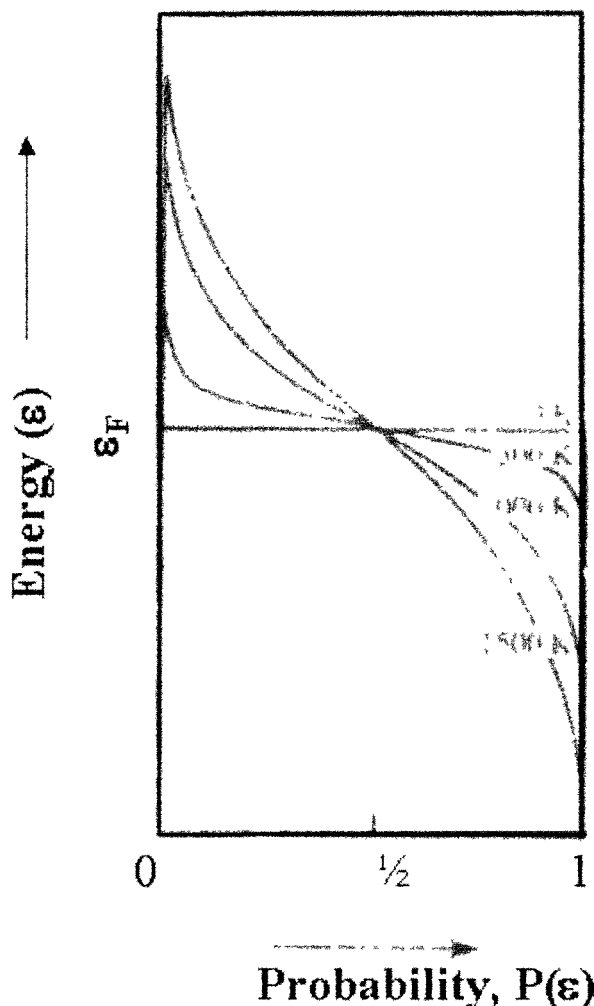


Fig. 1.8 The probability of filling is a function of energy level and temperature. The probability of filling at the Fermi energy is $\frac{1}{2}$ for all temperatures. As T increases $P(\epsilon)$ extends to higher energies.

The amorphous semi-conductor is different from the normal semi-conductor because impurities do not substantially affect the conductivity of the former. The weak dependence of conductivity on impurity is explained on the basis that large fluctuations exist in the local arrangement of atoms. This in turn will provide a large number of localized trap levels, and impurity or not, there is not much difference in conductivity. Considering the electron traps, we distinguish between shallow traps closer to the conduction band, and deep traps closer to the valence band. The electrons in shallow traps have approximately the same energy as those in the conduction band and are likely to be thermally excited in to that band. Electrons in the ground state, however, are more likely to recombine with a free hole rather than be re-excited to the conduction band (fig.

1.9). The recombination time may be relatively long. Thus electrons in the ground state act as though they are deep traps and recombination centers.

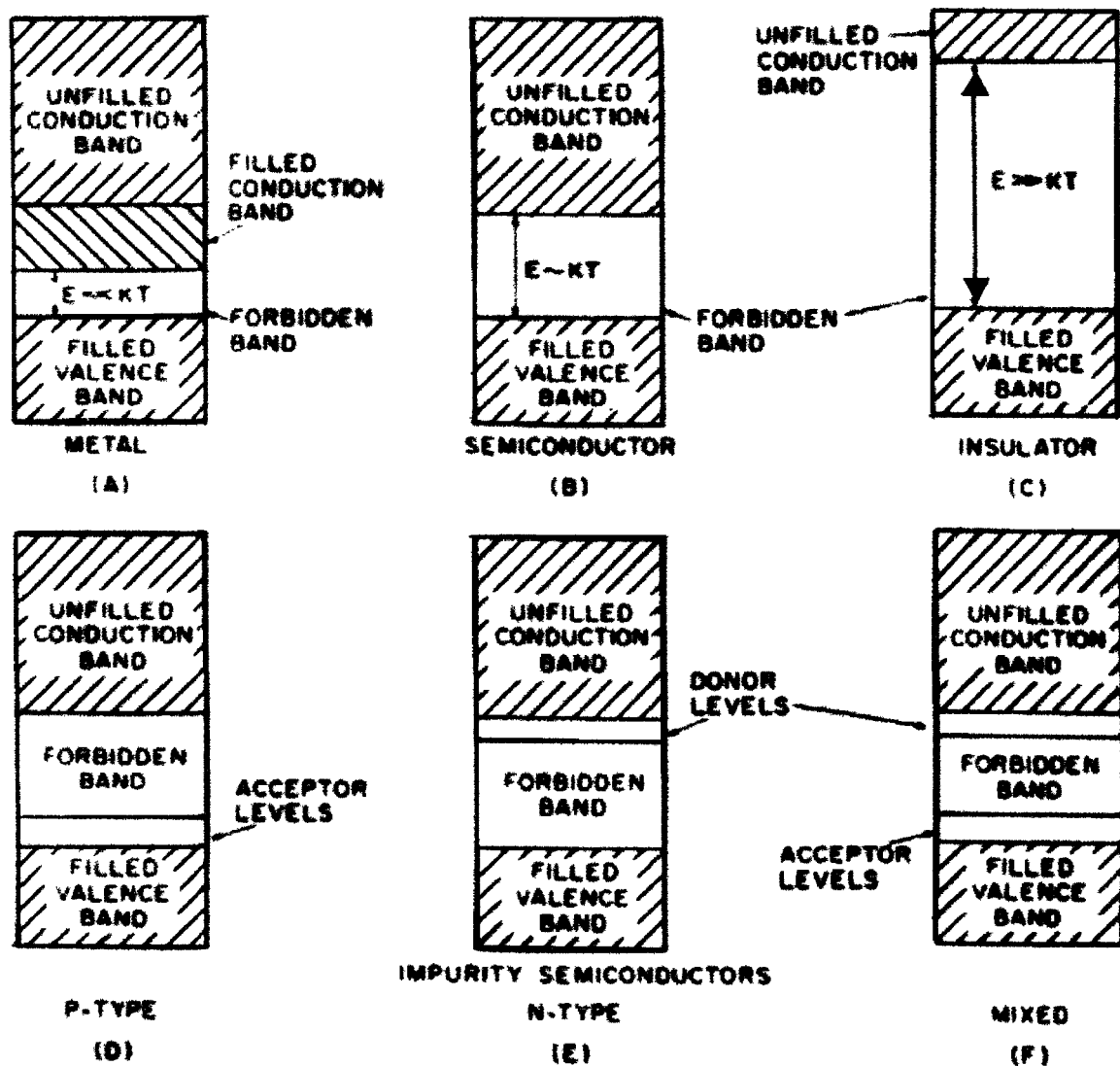


Fig. 1.9 Band theory for conduction in metals, semi-conductors, and Insulators [After A. H. Wilson, Proc. Roy. Soc., A 133 (1931) 458] (with permission of the Royal Society).

Shallow traps and the ground states are separated by an energy level which corresponds to the Fermi level in the excited state. This level is the steady-state under excitation. To distinguish this level from the Fermi level corresponding to that in the metal the term 'dark Fermi level' has been used (Eckertova, 1990). Electrons in the Fermi level have the same probability of being excited to the conduction band or falling into the ground state. Free electrons in the conduction band and free holes in the valence band can move under the influence of an electric field, though the mobility of the electrons is much

higher. Electrons can also transfer between localized states, eventually ending up in the conduction band. This process is known as “conduction by hopping”. An electron transferring from a trap to another localized state under the influence of an electric field is known as the Poole-Frenkel effect. Fig. 1.11^{5, 6} shows the various possible levels for both the electrons and the holes.

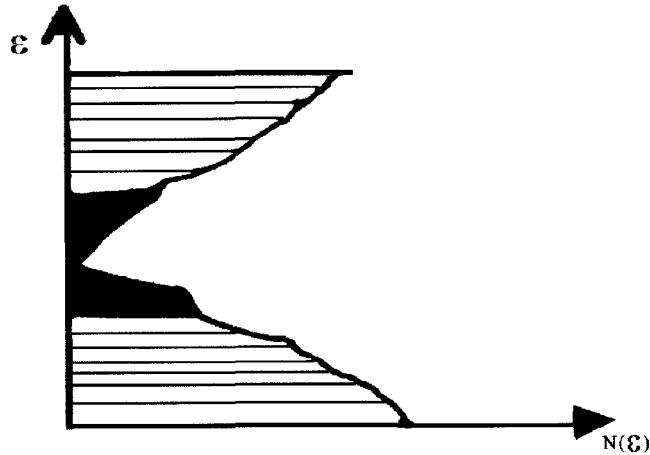


Fig. 1.10 Energy diagram of an amorphous material with the valence band and conduction band having rough edges (Schematic diagram).

1.6.3 ELECTRON EMISSION FROM A METAL

Electrons can be released from a metal by acquiring energy from an external source. The energy may be in the form of heat, by rising the temperature or by electromagnetic radiation. The following mechanisms may be distinguished:

(1) Thermionic Emission (Richardson-Dushman equation):

$$J = (1 - R) B_0 T^2 \exp\left(-\frac{\phi}{kT}\right); \quad B_0 = \frac{4\pi emk^2}{h^3} \quad (1.84)$$

where J is the current density, ϕ the work function, T the absolute temperature and R the reflection co-efficient of the electron at the surface. The value of R will depend upon the surface conditions. B_0 , called the Richardson-Dushman constant, has a value of $1.20 \times 10^6 \text{ A m}^{-2} \text{ K}^{-2}$. The term $(1-R)B_0$ can be as low as $1 \times 10^2 \text{ A m}^{-2} \text{ K}^{-2}$.

(2) Field assisted thermionic emission (Schottky equation):

In the presence of a strong electric field the work function is reduced according to

$$\phi_{\text{eff}} = \phi - \left[\frac{e^3 E}{4\pi\epsilon_0} \right]^{1/2} \quad (1.85)$$

where ϵ_0 is the permittivity of free space = 8.854×10^{-12} F/m and E the electric field. The current density is given by:

$$J = B_0 T^2 \exp \left[-\frac{(\phi - \beta_s E^{1/2})}{kT} \right]; \quad \beta_s = \left[\frac{e^3}{4\pi\epsilon_0} \right]^{1/2} \quad (1.86)$$

where and β_s , called the Schottky co-efficient, has a value of 3.79×10^{-5} [eV/ ($\text{V}^{1/2} \text{ m}^{-1/2}$)]

(3) Field emission (Fowler Nordheim equation)

In strong electric fields tunneling can occur even at room temperature and the current density for field emission is given by the expression:⁷

$$J = \frac{e^3 E^2}{8\pi h \phi} \exp \left\{ -\frac{4 \left(\frac{2m}{h^2} \right)^{\frac{1}{2}} (\phi - E_F)^{\frac{1}{2}}}{eE} \right\} \quad (1.87)$$

where J is the current density in A/m^2 , e the electronic charge in Coulomb, E is the electric field in V/m, h the Planck's constant in eV, ϕ the work function in eV and m the electron rest mass.

For practical applications equation (1.87) may be simplified to

$$I_{FN} = C_3 E^2 \exp \left(-\frac{C_4}{E} \right) \quad (1.88)$$

Improvements have been worked out to this equation but it is accurate enough for our purposes.

The effect of temperature is to multiply the current density by a factor:

$$\frac{f(\phi)T}{\sin[f(\phi)T]} \quad (1.89)$$

where

$$f(\phi) = \frac{2\pi k(2m^* \phi)^2}{\hbar e E} \quad (1.90)$$

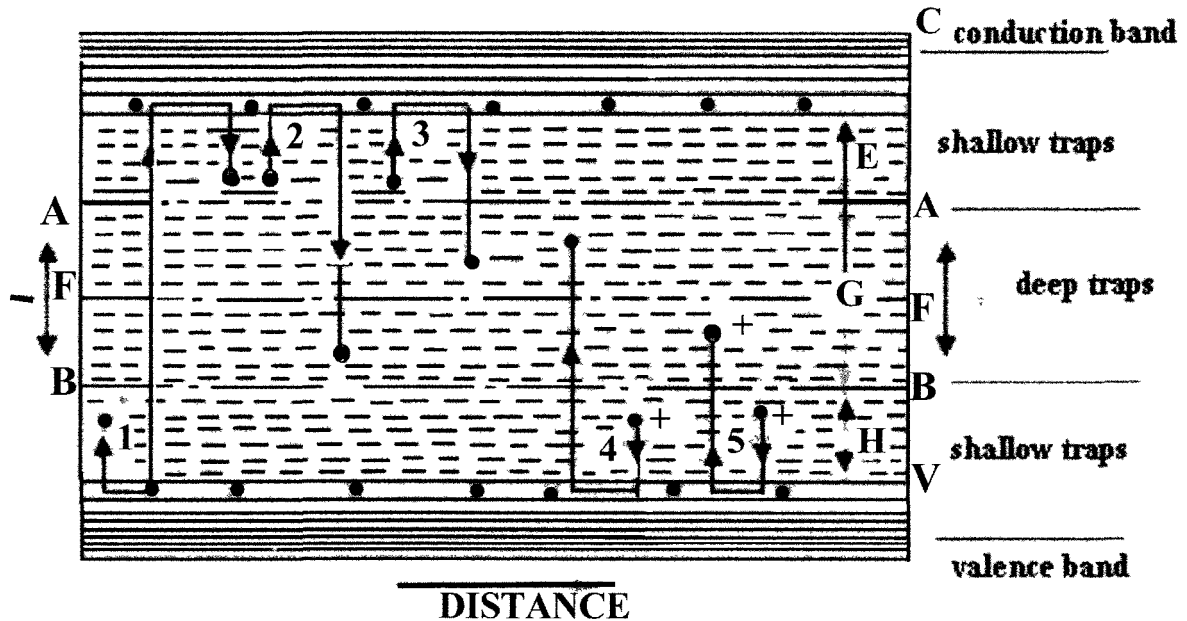


Fig. 1.11 Band-gap model and trapping events. C: conduction band, V: valence band, F-F: dark Fermi level, A-A: electron Fermi level (under photo-excitation), B-B: hole Fermi level (under photo-excitation), E: shallow electron traps, H: shallow hole traps, G: ground states (retrapping centers, deep traps), 1: photoexcitation of molecule; hole is captured in neutral shallow trap; electron is lifted to conduction band and captured in shallow electron trap; 2: shallow trapped electron is thermally activated into the conduction band, recombines into ground state; 3-shallow trapped electron, thermally activated into conduction band, is captured by deep trap; 4-4-shallow trapped hole receives electron from valence band and recombines into ground state; 5: shallow trapped hole receives electron from ground state and is captured in deep trap. The figure shows carrier movement under an applied electric field (Johnson, 1972; with permission of IEEE ©).

Here m^* is the effective rest mass of the electron. The temperature correction for the field emission current is small and given in Table 1.1.

Table 1.1
Temperature correction for the field emission current^{8b}

T(K)	MULTIPLYING FACTOR			
	$\phi=1$ eV	$\phi=2$ eV	$\phi=3$ eV	$\phi=4$ eV
100	1.013	1.026	1.040	1.067
200	1.053	1.111	1.172	1.312
300	1.126	1.275	1.454	1.943
400	1.239	1.570	2.048	4.050
500	1.411	2.123	3.570	

1.6.4 FIELD INTENSIFICATION FACTOR

The electric field at the cathode is a macroscopic field and hence an average field at all points on the surface. It is idealized assuming that the cathode surface is perfectly smooth which is impossible to realize in practice. The surface will have imperfections and the electric field at the tip of these micro-projections will be more intense depending upon the tip radius; the smaller the radius, that is, the sharper the micro-projection greater will be the electric field at the tip. The effect of a micro-projection may be taken into account by introducing a field intensification factor β . The field emission current may now be expressed as:

$$\ln\left(\frac{I_{FN}}{E^2}\right) = \ln K_3 + \ln A + 2\ln\beta - \frac{C_4}{\beta E} \quad (1.91)$$

We see that a plot of $\ln\left(\frac{I_{FN}}{E^2}\right)$ against $1/E$ yields a straight line from the slope of which β may be calculated. The field intensification factor depends upon the ratio h/r where h is the height and r the radius of the projection. Experimentally observed values of β can be as high as 1000^9 .

Recent measurements on electron emission in a vacuum have been carried out by Juttner et. al.^{10, 11} with a time resolution of 100 ns and the vacuum gap exposed to a second gap in which high current arcing $\sim 15A$ occurs. Higher emission currents are observed with a time constant of 1-3 μs and mechanical shocks are also observed to increase emission.

Field emission from atomic structures that migrate to the surface under the influence of the electric field is believed to increase the emission current, which renders the spark breakdown of the vacuum gap lower. Mechanical shocks are also believed to increase the migration, explaining the observed results.

1.7 ENERGY DISTRIBUTION FUNCTION

We consider now the distribution of energies of particles in a gas. A detailed discussion of energy distribution of electrons is given in chapter 9 and the present discussion is a simplified approach because inelastic collisions, which result in energy loss, are neglected. The energy distribution of molecules in a gas is given by the well known Maxwell distribution or Boltzmann distribution. The velocity distribution function according to Maxwell is given by

$$f(v) = \frac{4}{\pi^2} \left(\frac{m}{2kT} \right)^{\frac{3}{2}} v^2 \exp \left[-\frac{mv^2}{2kT} \right] \quad (1.92)$$

The arithmetic mean speed which is also called the **mean thermal velocity** v_{th} is given by

$$v_{th} = \left(\frac{8kT}{\pi m} \right)^{\frac{1}{2}} \quad (1.93)$$

The velocity distribution is expressed in terms of the energy by substituting

$$\varepsilon = \frac{1}{2}mv^2$$

However the Maxwell distribution may be considered as a particular case of a general distribution function of the form¹²

$$F(\varepsilon)d\varepsilon = A \frac{\varepsilon^{\frac{1}{2}}}{\bar{\varepsilon}^{\frac{3}{2}}} \exp \left[-B \left(\frac{\varepsilon}{\bar{\varepsilon}} \right)^{2(p+1)} \right] \quad (1.94)$$

in which $\bar{\varepsilon}$ is the mean energy of the electrons and, A and B are expressed by the following functions.

$$A = 2(p+1) \left[\Gamma \frac{5}{4(p+1)} \right]^{3/2} \times \left[\Gamma \frac{3}{4(p+1)} \right]^{-5/2} \quad (1.95)$$

$$B = \left[\Gamma \frac{5}{4(p+1)} / \Gamma \frac{3}{4(p+1)} \right]^{2(p+1)} \quad (1.96)$$

in which the symbol Γ stands for **Gamma function**. The Gamma function is defined according to

$$\Gamma(n+1) = n! = 1 \cdot 2 \cdot 3 \cdot \dots \cdot (n-1) \cdot n$$

$$\Gamma(n+1) = n\Gamma n$$

Some values of the gamma functions are:

$$\Gamma \frac{1}{4} = 3.6256; \quad \Gamma \frac{1}{3} = 2.6789; \quad \Gamma \frac{1}{2} = 1.7724; \quad \Gamma \frac{3}{4} = 1.2254$$

Values of the Gamma function are tabulated in Abramowitz and Stegun¹³. The energy distribution function given by the expression (1.94) is known as the p-set^{14, 15} and is quite simple to use. $p = -1/2$ gives the Maxwellian distribution identical to (1.92), the difference being that the latter expression is expressed in terms of the temperature T. The distribution functions for various values of p are shown in figure (1.12) for a mean energy of 4 eV. The use of the distribution function for calculating the swarm properties of the electron avalanche will be demonstrated in chapter 8.

1.8 THE BOLTZMANN FACTOR

We adopt a relatively easy procedure to derive the Boltzmann factor for a gas with equilibrium at a uniform absolute temperature T ². Consider a large number of similar particles which interact weakly with each other. Gas molecules in a container are a typical example. It is not necessary that all particles be identical, but if they are not identical, then there must be a large number of each species. Electrons in a gas may be a typical example. We shall derive the probability that a molecule has an energy E. Suppose that the molecules can assume energy values in the ascending values $E_1, E_2,$

$E_3, \dots E_n$. The energy may vary discreetly or continuously as in the case of ideal gas molecules. In either case we assume that there are no restrictions on the number of molecules that can assume a given energy E_n .

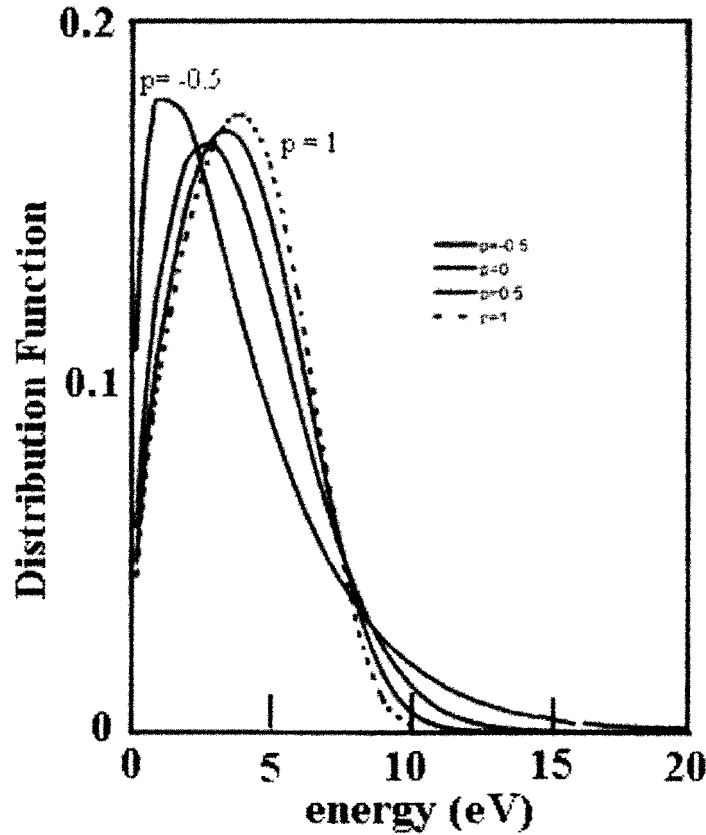


Fig. 1.12 Energy distribution function for various values of p for mean energy of 4 eV. $p = -0.5$ gives Maxwellian distribution (author's calculation).

Let us consider two particles with energy E_1 and E_2 before collision, and their energy becomes E_3 and E_4 , respectively, after collision. Conservation of energy dictates that

$$E_1 + E_2 \Leftrightarrow E_3 + E_4 \quad (1.97)$$

where the symbol $\Leftrightarrow$ means that the equality holds irrespective of which side is before and after the event of collision. In equilibrium condition let the probability of an electron having an energy E be $P(E)$ where $P(E)$ is the fraction of electrons with energy E . The probability of collision between two particles of energies E_1 and E_2 is $P(E_1) P(E_2)$. After collision the energies of the two particles are E_3 and E_4 (Fig. 1.13). The probability of collision is $P(E_3) P(E_4)$. The probability of collisions from left to right should be equal to the probability of collisions from right to left.

$$P(E_1)P(E_2) = P(E_3)P(E_4) \quad (1.98)$$

The solution of equations (1.97) and (1.98) is

$$P = A \exp(-E/kT) \quad (1.99)$$

where A is a constant. Equation (1.99) is perhaps one of the most fundamental equations of classical physics. Instead of assuming that all particles are of the same kind, we could consider two different kinds of particles, say electrons and gas molecules. By a similar analysis we would have obtained the same constant k for each species. It is therefore called the universal **Boltzmann constant** with a value of $k = 1.381 \times 10^{-23} \text{ J/K} = 8.617 \times 10^{-5} \text{ eV/K}$.

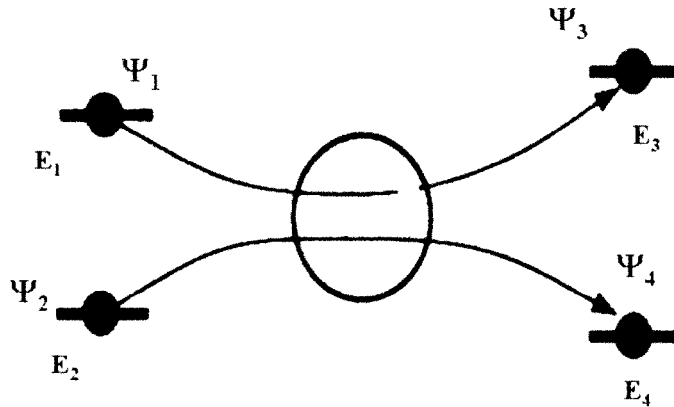


Fig. 1.13 Particles of wave functions Ψ_1 and Ψ_2 interact and end up with energies E_3 and E_4 . Their corresponding wave functions are Ψ_3 and Ψ_4 (Kasap, 1997). (with permission of McGraw Hill Co.,)

1.9 A COMPARISON OF DISTRIBUTION FUNCTIONS

The Boltzmann distribution function given by equation (1.99), n/N_c , does not impose any restriction on the number of molecules or electrons having the same energy, except that the number should be large. However, in quantum electronics, Pauli's exclusion principle forbids two electrons having the same energy and one adopts the Fermi distribution (equation (1.83)) instead. The differences between the two distribution functions are shown in Table 1.2.

Table 1.2
Comparison of Boltzmann and Fermi Distributions
Extracted from Ref. ¹⁶ (with permission)

	Boltzmann	Fermi
Distribution Function	$A \exp (-E/kT)$	$\{\text{Exp}[(E-E_F)/kT]+1\}^{-1}$
Basic characteristic.	Applies to distinguishable particles	Applies to indistinguishable particles obeying the exclusion principle.
Example of system.	Distinguishable particles or approximation to quantum distribution at $E \gg kT$	Identical particles of odd half integral spin.
Behavior of the distribution function.	Exponential function of E/kT	For $E \gg kT$, exponential where $E \gg E_F$. If $E_F \gg kT$, decreases abruptly near E_F .
Specific problems applied to in this book.	Distribution of dipoles in ch. 2; Energy distribution of electrons in Ch. 8	Electrons in dielectrics, Ch. 1, Ch.7-12.

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